

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

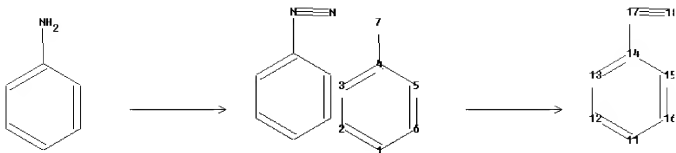
LOGINID:SSPTAKAB1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	3	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	4	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	5	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	6	JUN 25	CA/CAPLUS and USPAT databases updated with IPC reclassification data
NEWS	7	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS	8	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS	9	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS	10	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS	11	JUL 28	CA/CAPLUS patent coverage enhanced
NEWS	12	JUL 28	EPFULL enhanced with additional legal status information from the EPOline Register
NEWS	13	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	14	JUL 28	STN Viewer performance improved
NEWS	15	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	16	AUG 13	CA/CAPLUS enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	17	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	18	AUG 15	CAPLUS currency for Korean patents enhanced
NEWS	19	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS	20	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS	21	SEP 25	CA/CAPLUS current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS	22	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and Korean patents enhanced
NEWS	23	SEP 29	IFICLS enhanced with new super search field
NEWS	24	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS	25	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents



```

chain nodes :
7 17 18
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 16
chain bonds :
4-7 14-17 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
exact/norm bonds :
4-7 14-17 17-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
isolated ring systems :
containing 1 : 11 :

```

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 11:Atom 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS
fragments assigned reactant/reagent role:
containing 1
containing 11

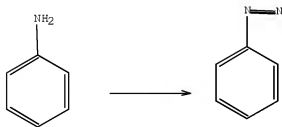
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L1 STRUCTURE UPLOADED

=> d L1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> file casreact
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.46	0.67

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 18 Oct 2008 VOL 149 ISS 17

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 15.3 million reactions
*
*
*****
```

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L1 SSS full

FULL SEARCH INITIATED 10:01:17 FILE 'CASREACT'
SCREENING COMPLETE - 22603 REACTIONS TO VERIFY FROM 2507 DOCUMENTS
100.0% DONE 22603 VERIFIED 1129 HIT RXNS 177 DOCS
SEARCH TIME: 00.00.05

L2 177 SEA SSS FUL L1 (1129 REACTIONS)

=> s L2 AND (diazonium salt)

2459 DIAZONIUM
52705 SALT
886 DIAZONIUM SALT
(DIAZONIUM(W)SALT)
L3 15 L2 AND (DIAZONIUM SALT)

=> d ibib abs hitstr 1-

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE, Single-step Reactions
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data

CAN ----- List of CA abstract numbers without answer numbers
 CBIB ----- AN, plus Compressed Bibliographic Data
 DALL ----- ALL, delimited (end of each field identified)
 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IND ----- Indexing data
 IPC ----- International Patent Classifications
 ISTD ----- STD, indented with text labels
 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

 MAX ----- Same as ALL
 PATS ----- PI, SO
 SCAN ----- TI and FCRD (random display, no answer number. SCAN
 must be entered on the same line as DISPLAY, e.g.,
 D SCAN.)
 SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for
 all single-step reactions)
 STD ----- BIB, IPC, and NCL

 CRD ----- Compact Display of All Hit Reactions
 CRDREF ----- Compact Reaction Display and SO, PY for Reference
 FHIT ----- Reaction Map, Diagram, and Summary for first
 hit reaction
 FHITCBIB --- FHIT, AN plus CBIB
 FCRD ----- First hit in Compact Reaction Display (CRD) format
 FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
 CA reference information (SO, PY). (Default)
 FPATH ----- PATH, plus Reaction Summary for the "long path"
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"
 HIT ----- Reaction Map, Reaction Diagram, and Reaction
 Summary for all hit reactions and fields containing
 hit terms
 OCC ----- All hit fields and the number of occurrences of the
 hit terms in each field. Includes total number of
 HIT, PATH, SPATH reactions. Labels reactions that have
 incomplete verifications.
 PATH ----- Reaction Map and Reaction Diagram for the "long
 path". Displays all hit reactions, except those
 whose steps are totally included within another hit
 reaction which is displayed
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)
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 multistep reactions that have a hit substance in both
 the first and last steps of the reaction, except for
 those hit reactions whose steps are totally included
 within another hit reaction which is displayed

To display a particular field or fields, enter the display field
 codes. For a list of the display field codes, enter HELP DFIELDS
 at an arrow prompt (=>). Examples of combinations include: D TI;

D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008)

L1 FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008
STRUCTURE UPLOADED

L2 FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008
177 S L1 SSS FULL
L3 15 S L2 AND (DIAZONIUM SALT)

=> d ibib abs hitstr 1-

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CBIB ----- AN, plus Compressed Bibliographic Data
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IND ----- Indexing data
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SIBIB ----- IBIB, no citations

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D SCAN.)
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 as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,
 FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
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ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008)

FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008

L1 STRUCTURE UPLOADED

FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008

L2 177 S L1 SSS FULL

L3 15 S L2 AND (DIAZONIUM SALT)

=> s L3

2459 DIAZONIUM

52705 SALT

886 DIAZONIUM SALT

(DIAZONIUM(W)SALT)

L4 15 L2 AND (DIAZONIUM SALT)

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'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

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 STD ----- BIB, IPC, and NCL

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 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)
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 those hit reactions whose steps are totally included
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ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008)

FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008

L1 STRUCTURE UPLOADED

FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008

L2 177 S L1 SSS FULL

L3 15 S L2 AND (DIAZONIUM SALT)

L4 15 S L3

=> d ibib abs fhit

L4 ANSWER 1 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 147:72477 CASREACT Full-text

TITLE: Synthesis and structure of some azo coupled cyclic β -enaminones

AUTHOR(S): Simunek, Petr; Luskova, Lucie; Svobodova, Marketa; Bertolasi, Valerio; Lycka, Antonin; Machacek, Vladimir
CORPORATE SOURCE: Department of Organic Chemistry, University of Pardubice, Pardubice, CZ-532 10, Czech Rep.

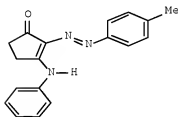
SOURCE: Magnetic Resonance in Chemistry (2007), 45(4), 330-339
CODEN: MRCHEG; ISSN: 0749-1581

PUBLISHER: John Wiley & Sons Ltd.

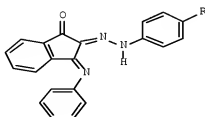
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

AB The reaction of 3-phenylaminocyclopent-2-en-1-one with 4-Me, 4-methoxy and 4-chlorobenzenediazonium tetrafluoroborates was used to prepare the azo coupling products, e.g., I. It was found that these compds. are present in both CDC13 solution and solid phase practically exclusively as (E)-3-phenylamino-2-(4-

subst.phenyldiazenyl)cyclopent-2-en-1-ones with N-H...N intramol. hydrogen bond. The substitution of the Ph residue of the diazonium salt has no effect on the position of the tautomeric equilibrium. On the other hand, the compds. (II; R = Me or H) formed by the reaction of 3-phenylamino-1H-inden-1-one with 4-methylbenzene- or benzenediazonium tetrafluoroborates exist in CDCl₃ solution and in solid phase as hydrazone compds. In the solution they occur as a mixture of three forms, out of which two were identified as E/Z isomers with different types of hydrogen bonds. The compound formed by the reaction of 3-amino-5,5-dimethylcyclohex-2-en-1-one with 4-methoxybenzenediazonium tetrafluoroborate is converted into a stable hydrochloride on standing in CHCl₃ solution; this product exhibits a high degree of delocalization of the pos. charge. Its structure was studied by means of X-ray.

RX(9) OF 14 COMPOSED OF RX(1), RX(3)
RX(9) A + E + J ==> K



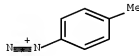
A



B

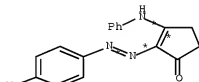


J: CM 1



J: CM 2

2
STEPS
→



K
YIELD 26%

RX(1) RCT A 3859-41-4, B 62-53-3
PRO C 73825-35-1
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 4 hours, reflux
SUBSTAGE(2) cooled

RX(3) RCT C 73825-35-1, J 459-44-9
RGT L 127-09-3 AcONa
PRO K 941717-55-1
SOL 75-09-2 CH2Cl2
CON 24 hours, room temperature
NTE stereoselective

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs fhit 1-

YOU HAVE REQUESTED DATA FROM 15 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 147:72477 CASREACT [Full-text](#)

TITLE: Synthesis and structure of some azo coupled cyclic β -enaminones

AUTHOR(S): Simunek, Petr; Luskova, Lucie; Svobodova, Marketa; Bertolasi, Valerio; Lycka, Antonin; Machacek, Vladimir
CORPORATE SOURCE: Department of Organic Chemistry, University of Pardubice, Pardubice, CZ-532 10, Czech Rep.

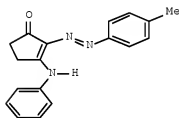
SOURCE: Magnetic Resonance in Chemistry (2007), 45(4), 330-339
CODEN: MRCHEG; ISSN: 0749-1581

PUBLISHER: John Wiley & Sons Ltd.

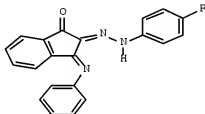
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I



II

AB The reaction of 3-phenylaminocyclopent-2-en-1-one with 4-Me, 4-methoxy and 4-chlorobenzenediazonium tetrafluoroborates was used to prepare the azo coupling products, e.g., I. It was found that these compds. are present in both CDCl₃ solution and solid phase practically exclusively as (E)-3-phenylamino-2-(4-subst.phenyldiazenyl)cyclopent-2-en-1-ones with N-H...N intramol. hydrogen bond. The substitution of the Ph residue of the diazonium salt has no effect on the position of the tautomeric equilibrium. On the other hand, the compds. (II; R = Me or H) formed by the reaction of 3-phenylamino-1H-inden-1-one with 4-methylbenzene- or benzenediazonium tetrafluoroborates exist in CDCl₃ solution and in solid phase as hydrazone compds. In the solution they occur as a mixture of three forms, out of which two were identified as E/Z isomers with different types of hydrogen bonds. The compound formed by the reaction of 3-amino-5,5-dimethylcyclohex-2-en-1-one with 4-methoxybenzenediazonium tetrafluoroborate is converted into a stable hydrochloride on standing in CHCl₃ solution; this product exhibits a high degree of delocalization of the pos. charge. Its structure was studied by means of X-ray.

RX(9) OF 14 COMPOSED OF RX(1), RX(3)

RX(9) A + B + J ==> K



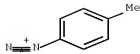
A



B

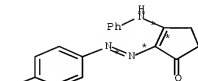


J: CM 1



J: CM 2

2
STEPS
→



K
YIELD 26%

RX(1) RCT A 3859-41-4, B 62-53-3
PRO C 73825-35-1
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 4 hours, reflux
SUBSTAGE(2) cooled

RX(3) RCT C 73825-35-1, J 459-44-9
RGT L 127-09-3 AcONa
PRO K 941717-55-1
SOL 75-09-2 CH2Cl2
CON 24 hours, room temperature
NTE stereoselective

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 143:459818 CASREACT Full-text

TITLE: 2-Methoxy-4-nitrobenzenediazonium salt as a practical diazonium-transfer agent for primary arylamines via tautomerism of 1,3-diaryltriazenes: Deaminative iodination and arylation of arylamines without direct diazotization

AUTHOR(S): Saeki, Tomoyuki; Son, Eun-Cheol; Tamao, Kohei
CORPORATE SOURCE: International Research Center for Elements Science, Institute for Chemical Research, Kyoto University, Uji, Japan

SOURCE: Bulletin of the Chemical Society of Japan (2005), 78(9), 1654-1658
CODEN: BCSJAB; ISSN: 0009-2673

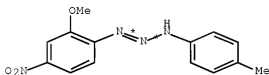
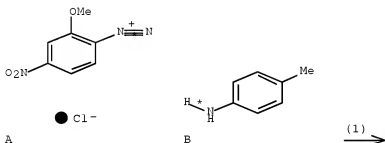
PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1,3-Diaryltriazenes, prepared from a 2-methoxy-4-nitrobenzenediazonium salt and primary arylamines, exist as azo-transfer tautomers in which the 2-methoxy-4-nitrophenyl group is present on the saturated nitrogen atom and forms a hydrogen bond between the 2-methoxy group and the N-H moiety. The synthetic utility of the diazonium salt as a practical diazonium-transfer agent for primary arylamines via tautomerism of the 1,3-diaryltriazenes has been demonstrated by the deaminative iodination and arylation of the arylamines without direct diazotization. The starting 2-methoxy-4-nitrophenylamine can be easily recovered after the reactions.

RX(1) OF 37 A + B ==> C...



C
YIELD 70%

RX(1) RCT A 120-17-2, B 106-49-0
RGT D 584-08-7 K2CO3
PRO C 869373-61-5
CON 30 minutes, 0 deg C

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 143:440299 CASREACT [Full-text](#)

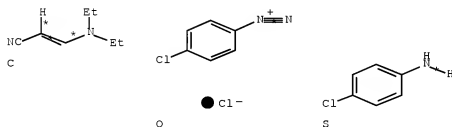
TITLE: Studies with functionally substituted enamines:
synthesis of new aminoazolo-pyrimidines and
-1,2,4-triazines

AUTHOR(S): Ghozlan, Said Ahmed Soliman; Abdelhamid, Ismail
Abdelshafy; Gaber, Hatem; Elnagdi, Mohamed Hilmy

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Cairo
University, Giza, Egypt

SOURCE: Journal of Chemical Research (2004), (12), 789-793
 CODEN: JCROA4
 PUBLISHER: Science Reviews
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 3-Aminoacrylonitrile derivs., R1R2NCH:CHCN (R1 = R2 = Et (1d), Ph (1e), (CH2)5 (1f), (CH2CH2)2O (1g)) coupled with aromatic and heteroarom. diazonium salts yielding arylhydrazonals and pyrazolo[5,1-c]triazines. The enaminonitriles 1 condensed to form dienes on reflux in acetic acid. The latter underwent Diels-Alder type addition to naphthoquinone. Aminopyrazolopyrimidines were obtained from reaction of 1d-1g with heteroarom. aminoazoles. Enaminonitrile 1d formed pyran with benzylidenemalononitrile, and dihydropyrimidine with benzaldehyde and urea.

RX(47) OF 57 COMPOSED OF RX(6), RX(8)
 RX(47) C + O + S ==> T



RX(6) RCT C 58243-06-4, O 2028-74-2
 RGT M 127-09-3 AcONa
 PRO P 849820-80-0
 SOL 64-19-7 AcOH
 CON 1 hour, room temperature

RX(8) RCT S 106-47-8

STAGE(1)
 RGT U 7647-01-0 HCl, V 7632-00-0 NaNO2
 SOL 7732-18-5 Water
 CON room temperature

STAGE(2)

RCT P 849820-80-0
 RGT M 127-09-3 AcONa
 SOL 64-17-5 EtOH
 CON room temperature

PRO T 7071-45-6

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

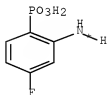
ACCESSION NUMBER: 143:286545 CASREACT [Full-text](#)
 TITLE: Synthesis of fluorophosphonoazo derivative as color
 reagent for thorium
 INVENTOR(S): Wu, Bincai; Wang, Bing
 PATENT ASSIGNEE(S): East China Normal University, Peop. Rep. China
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 9 pp.
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1450071	A	20031022	CN 2003-116907	20030514
PRIORITY APPLN. INFO.:			CN 2003-116907	20030514

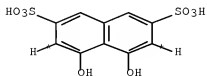
AB The title compound, 2-(5-fluoro-2-phosphonophenylazo)-7-(3-fluorophenylazo)-1,8-dihydroxy-3,6-naphthalenedisulfonic acid, is synthesized by nitrifying 4-fluoroaniline with fuming HNO₃/glacial acetic acid in glacial acetic acid/acetic anhydride to obtain 4-fluoro-2-nitroaniline, diazotizing with NaNO₂ in HCl solution and then salifying with NaBF₄, reducing and substituting with PCl₃ in Et acetate in the presence of CuCl, hydrolyzing with water to obtain 2-amino-4-fluorophenylphosphonic acid, diazotizing, coupling with chromotropic acid Na salt, and then coupling with diazonium salt of 4-fluoroaniline. Th(IV) is determined by spectrophotometry at 680 nm in 6M HCl medium with m-fluoroazofluorophosphine as color developing agent and 1-butanol as extractant.

RX(9) OF 15 COMPOSED OF RX(4), RX(5)

RX(9) M + Q + T ==> U



M

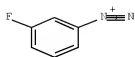


Q

● 2 Na

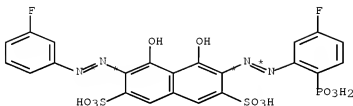


T: CM 1



T: CM 2

2
STEPS
→



U

RX(4) RCT M 648863-06-9

STAGE(1)

RGT I 7632-00-0 NaNO₂, J 7647-01-0 HCl

SOL 7732-18-5 Water

CON 0.5 hours, 0 deg C

STAGE(2)

RCT Q 129-96-4

RGT S 127-09-3 AcONa

SOL 7732-18-5 Water

CON 1 hour, 10 deg C

STAGE(3)

RGT J 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH <1

PRO R 681145-02-8

RX(5) RCT R 681145-02-8, T 1996-38-9

STAGE(1)

RGT V 1310-65-2 LiOH

SOL 7732-18-5 Water

CON 1 hour, 0 deg C, pH 8 - 10

STAGE(2)

RGT W 12408-02-5 H+

SOL 7732-18-5 Water

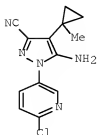
PRO U 864380-51-8

L4 ANSWER 5 OF 15 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 142:316832 CASREACT Full-text
 TITLE: Process for the preparation of substituted aryl
 pyrazoles via cyclization of diazo compounds with
 2,3-dicyanopropionates and related derivatives
 INVENTOR(S): Gladwell, Iain Robert; Matthews, John George; Pettman,
 Alan John
 PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
 SOURCE: PCT Int. Appl., 69 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023773	A1	20050317	WO 2004-IB2758	20040824
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050096354	A1	20050505	US 2004-932390	20040902
PRIORITY APPLN. INFO.:			GB 2003-20719	20030904
			GB 2004-14893	20040702
			US 2003-517349P	20031104
			US 2004-600405P	20040809
OTHER SOURCE(S):			MARPAT 142:316832	
GI				



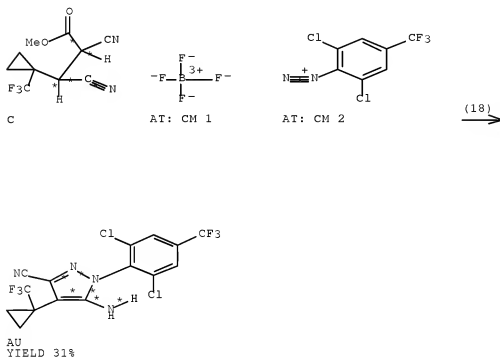
I



II

AB The invention is related to a process for the preparation of the well-known pesticides aminocyano 1-arylpyrazoles and 1-pyridinylpyrazoles of formula I via cyclization of aryldiazonium compds. $\text{Ar-N}^+\text{.tplbond.NX}^-$ (prepared in situ or isolated) with compds. of formula R3LCH-CHR1R5a , e.g. alkyl 2,3-dicyanopropionates, optionally in the presence of an acid [Ar = (un)substituted Ph, pyridinyl; R1 = (un)substituted alkyl, cycloalkyl, 5- or 6-membered heterocyclyl, cyclopropyl, fused bicycle, etc.; R3 = CN, CF3, CHO, COR, CO2R; R = (un)substituted alkyl; R5 = H, (un)substituted alkyl; R5a = CN, CO2H, CHO, COR, CO2R; L = activating group; X = compatible counter ion]. The advantages include improved product yield, lower reaction time, and reduced number of steps. Thus, reacting Me 2,3-dicyano-3-(1-methylcyclopropyl)propanoate (preparation given) with 6-chloropyridine-3-diazonium BF_4^- (preparation given) in MeCN at 0° for 20 min and at room temperature for 3 h, followed by treatment of the reaction mixture with NH_4OH gave pyrazole II in 68% yield.

RX(18) OF 73 C + AT ==> AU



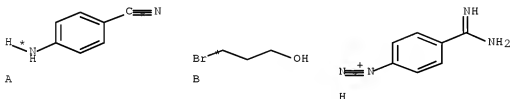
RX(18) RCT C 848074-26-0, AT 258353-28-5
 RGT AY 127-09-3 AcONa
 PRO AU 208937-91-1
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 15 minutes, cooled
 SUBSTAGE(3) 4.5 hours, room temperature
 NTE NaHCO_3 can also be used as base, sonication before the addition

of diazonium salt
 REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

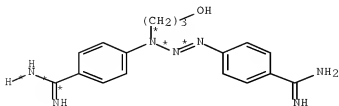
L4 ANSWER 6 OF 15 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 139:360542 CASREACT [Full-text](#)
 TITLE: Photochemical DNA cleavage by a Berenil analog
 AUTHOR(S): Burr, Sally J.; Mselati, Abdulghani; Thomas, Emrys W.
 CORPORATE SOURCE: Division of Biological Sciences, Salford University,
 Salford, M5 4WT, UK
 SOURCE: Tetrahedron Letters (2003), 44(39), 7307-7309
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Berenil [bis(4-aminophenyl)1,3-triazene] is a photostable DNA-binding ligand. We describe here the synthesis of N-(3-hydroxypropyl)-Berenil, which in contrast to Berenil is photosensitive to 360 nm irradiation, behaving as a caged diazonium salt. The 4-aminobenzenediazonium fragment produced by photolysis induces DNA modification and cleavage.

RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)
 RX(6) A + B + H ==> I



3
 STEPS
 →



I
 YIELD 50%

RX(1) RCT A 873-74-5, B 627-18-9
PRO C 313238-55-0
NTE no exptl. details

RX(2) RCT C 313238-55-0

STAGE(1)

RGT E 7647-01-0 HCl
SOL 67-56-1 MeOH

STAGE(2)

RGT F 7664-41-7 NH3
SOL 67-56-1 MeOH

PRO D 620947-05-9

RX(3) RCT D 620947-05-9, H 620947-06-0
PRO I 620947-07-1
NTE no exptl. details

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 139:214429 CASREACT [Full-text](#)

TITLE: Synthesis of azo-coupled itaconic acid anhydride and
its reactions with nucleophiles

AUTHOR(S): Prabhu, P. J.; Bhise, N. B.; Dave, M. A.

CORPORATE SOURCE: Department of Chemistry, K.J. Somaiya College of
Science and Commerce, Mumbai, 400 077, India

SOURCE: Asian Journal of Chemistry (2003), 15(2), 634-638
CODEN: AJCHEW; ISSN: 0970-7077

PUBLISHER: Asian Journal of Chemistry

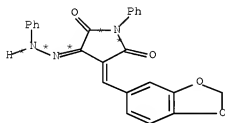
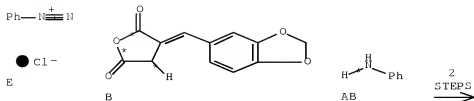
DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3,4-Methylenedioxy-benzylidene succinic anhydride was condensed with diazonium
salts of various aromatic amines to form hydrazones or dyes which were further
treated with nucleophiles like 10% NaOH and NaBH₄ to give various pyrazolinone
derivs., resp. and cyclic imide derivs. of the corresponding hydrazones. The
antibacterial and antifungal activities of some the products are also
reported.

RX(24) OF 45 COMPOSED OF RX(2), RX(14)

RX(24) E + B + AB ==> AC



RX(2) RCT E 100-34-5

STAGE(1)

RGT G 7647-01-0 HCl, H 7632-00-0 NaNO2
 SOL 7732-18-5 Water
 CON 15 minutes, 0 deg C

STAGE(2)

RCT B 99971-42-3
 SOL 67-64-1 Me2CO
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 30 minutes, 0 deg C

PRO F 587881-56-9

RX(14) RCT F 587881-56-9, AB 60-53-3

STAGE(1)

SOL 64-17-5 EtOH
 CON 4 - 5 hours, reflux

STAGE(2)

CAT 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature

PRO AC 587881-78-5

REFERENCE COUNT:

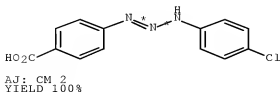
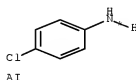
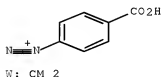
9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 137:124905 CASREACT [Full-text](#)
 TITLE: Waste-free chemistry of diazonium salts and benign separation of coupling products in solid salt reactions
 AUTHOR(S): Kaupp, Gerd; Herrmann, Andreas; Schmeyers, Jens
 CORPORATE SOURCE: Universitat Oldenburg FB Chemie, Organische Chemie I, Oldenburg, 26111, Germany
 SOURCE: Chemistry--A European Journal (2002), 8(6), 1395-1406
 CODEN: CEUJED; ISSN: 0947-6539
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Gas-solid and solid-solid techniques allow for waste-free and quant. syntheses in the chemical of diazonium salts. Five techniques for diazotations with the reactive gases NO₂, NO and NOCl are studied. Two types are mechanistically investigated with atomic force microscopy (AFM) and are interpreted on the basis of known crystal packings. The same principles apply to the cascade reactions that had been derived from one-step reactions. Solid diazonium salts couple quant. with solid diphenylamine and anilines to give the triazenes. Azo couplings are achieved with quant. yields by cautious co-grinding of solid diazonium salts with β -naphthol and C-H acidic heterocycles, such as barbituric acids or pyrazolinones. Solid diazonium salts may be more easily applied in a stoichiometric ratio for couplings in solution. Co-grinding of solid diazonium salts with KI gives quant. yields of various solid aryl iodides. The unavoidable coupling products in salt reactions are completely separated from the insol. products in a highly benign manner. The solid-state reactions compare favorably with similar solution reactions that produce much waste. The structures of the products are elucidated with IR and NMR spectroscopy and mass spectrometry, while the tautomeric properties of the compds. are studied with d. functional calcns. at the B3LYP/6-31G* and BLYP/6-31G** levels. Safety: care must be taken when handling solid diazonium salts.

RX(17) OF 51 W + AI ==> AJ...



RX(17) RCT W 178412-89-0, AI 106-47-8
 PRO AJ 444288-67-9
 NTE solid state, green chem.

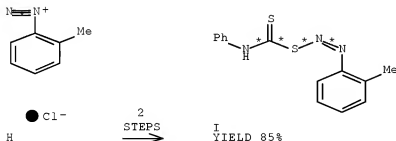
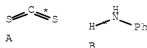
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 136:37382 CASREACT Full-text
 TITLE: Reactions of diazonium salts with phenyl dithiocarbamate. Part II. Formation of related arylazophenyldithiocarbamates
 AUTHOR(S): Haque, M. Zahurul; Ali, M. Umar; Ali, M. Hossen
 CORPORATE SOURCE: BCSIR Laboratories, Rajshahi, Bangladesh
 SOURCE: Journal of the Indian Chemical Society (2001), 78(7), 372-373
 CODEN: JICSAH; ISSN: 0019-4522
 PUBLISHER: Indian Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Reaction of 1-naphthyldiazonium salt with ammonium salt of phenyldithiocarbamic acid gives 1-naphthylazophenyldithiocarbamate. Similar reaction has been carried out with several other aryl diazonium chlorides. Antibacterial activity of the compds. has been evaluated.

RX(10) OF 15 COMPOSED OF RX(1), RX(3)
 RX(10) A + B + H ==> I



RX(1) RCT A 75-15-0, B 62-53-3
 RGT D 1336-21-6 NH4OH
 PRO C 1074-52-8
 SOL 7732-18-5 Water

RX(3) RCT C 1074-52-8, H 2028-34-4

PRO I 380149-05-3
SOL 7732-18-5 Water

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 134:353093 CASREACT Full-text

TITLE: Phenylene ethynylene diazonium salts as potential
self-assembling molecular devices

AUTHOR(S): Kosynkin, Dmitry V.; Tour, James M.

CORPORATE SOURCE: Department of Chemistry and Center for Nanoscale
Science and Technology, Rice University, Houston, TX,
77005, USA

SOURCE: Organic Letters (2001), 3(7), 993-995

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

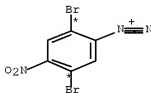
AB Functionalized diazonium salts for mol. electronic devices are prepared by the
reaction of the corresponding anilines with NOBF₄ in sulfolane-MeCN solvent.

RX(48) OF 133 COMPOSED OF RX(26), RX(1)

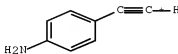
RX(48) 2 BJ + 3 B ==> C + D



2 BJ: CM 1

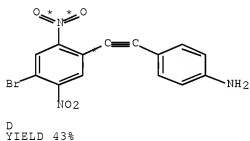
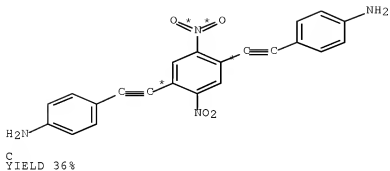


2 BJ: CM 2



3 B

2
STEPS
→



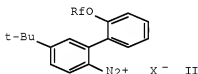
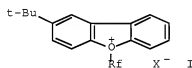
RX(26) RCT BJ 339175-69-8
RGT BK 7632-00-0 NaNO₂
PRO A 18908-08-2
SOL 7732-18-5 Water

RX(1) RCT A 18908-08-2, B 14235-81-5
RGT E 121-44-8 Et₃N
PRO C 339175-50-7, D 339175-70-1
CAT 13965-03-2 PdCl₂(PPh₃)₂, 7681-65-4 CuI
SOL 109-99-9 THF

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 15 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 130:168232 CASREACT [Full-text](#)
TITLE: Preparation of O-(perfluoroalkyl)dibenzofuranium salts as perfluoroalkylating agents and their intermediates such as (perfluoroalkoxy)biphenyldiazonium salts
INVENTOR(S): Umemoto, Teruo; Adachi, Kenji; Ishihara, Sumi
PATENT ASSIGNEE(S): Daikin Industries Ltd., Japan
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

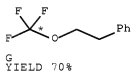
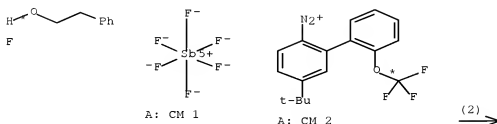
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906389	A1	19990211	WO 1998-JP3416	19980730
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1013651	A1	20000628	EP 1998-935301	19980730
EP 1013651	B1	20070530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 363477	T	20070615	AT 1998-935301	19980730
US 6239289	B1	20010529	US 2000-463706	20000215
PRIORITY APPLN. INFO.:			JP 1997-207901	19970801
			WO 1998-JP3416	19980730
OTHER SOURCE(S):			MARPAT 130:168232	
GI				



AB O-(Perfluoroalkyl)dibenzofuranium salt derivs. represented by general formula (I; Rf is perfluoroalkyl being 1 to 10 carbon atoms; and X- is a conjugate based of a Bronsted acid) are prepared by cyclization of (perfluoroalkoxy)biphenyldiazonium salts (II; Rf and X- are defined as above) and are used as perfluoroalkylating agents for perfluoroalkylation of nucleophiles containing O or N, e.g. amines and alcs. When the O-(perfluoroalkyl)dibenzofuranium salt derivs. are used as perfluoroalkylating agents, they permit high-yield perfluoroalkylation, and are applicable to a wide range of compds. and inhibited in self-decomposition as to be relatively stable. The presence of tert-Bu at 5-position improves the stability of I and thereby usefulness of I as perfluoroalkylating agents. Thus, a solution of 7.17 g 2-amino-5-tert-butyl-2'-(trifluoromethoxy)biphenyl in 46 mL Et2O was cooled to -78° with stirring, followed by adding 6.47 g nitrosonium hexafluoroantimonate (ON+SbF6-), and the resulting mixture was warmed to 10° over 3 h in an warm bath, while adding 10 mL Et2O when temperature reached to 5°, to give 58% II (Rf = CF3, X- = SbF6-) (III). A CCl2D2 solution of 6.5 mg III in a Pyrex NMR tube was cooled to -106° and irradiated by a high pressure Hg lamp (400 W and 253.7 nm) for 45 min to give I (Rf = CF3, X- = SbF6-) (IV) 87, 5-tert-butyl-2-fluoro-2'-(trifluoromethoxy)biphenyl 8, and 5-tert-butyl-2-chloro-2'-(trifluoromethoxy)biphenyl 3% according to 19F- and 1H-NMR anal. at -80°. When the temperature was gradually raised to -30°, IV completely decomposed to CF4 and 2-tert-butylbenzofuran. To the cold (-99° to -90°) reaction mixture similarly prepared were added variety of alcs. and amines. When phenetyl alc. was added at -90°, the resulting mixture was warmed to -10° over 3 h to give 80% phenetyl trifluoromethyl ether. Although in general, diazonium salts are explosive in nature, III has .apprx.27° higher

decomposition temperature (84.7-85.8°) compared to that of the 4-tert-Bu regioisomer (m.p. 58-60°) and can be handled at room temperature, and safely stored and transported.

RX(2) OF 9 F + A ==> G



RX(2) RCT F 60-12-8, A 220351-08-6

PRO G 175676-47-8

SOL 75-09-2 CH2Cl2

NTE two-step reaction involving in situ prepn. of
O-(trifluoromethyl)dibenzofuranium salt under irradiation of
(trifluoromethoxy)debenzofuran-2-diazonium
salt with a high pressure Hg lamp at -99° to
-90° for 70 min followed by trifluoromethylation at
-90° to -10° for 3 h

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 15 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 111:174247 CASREACT [Full-text](#)

TITLE: Reaction of tris(perfluoroalkyl)phosphine oxides and
tris(perfluoroalkyl)difluorophosphoranes with fluoroide
ion

AUTHOR(S): Pavlenko, N. V.; Yagupol'skii, L. M.

CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

SOURCE: Zhurnal Obshchei Khimii (1989), 59(3), 528-34

CODEN: ZOKHA4; ISSN: 0044-460X

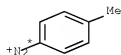
DOCUMENT TYPE: Journal

LANGUAGE: Russian

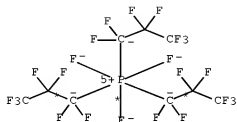
AB Treating (C2F5)3P(O) with 1 or 2 equivalent CsF in Et2O gave (C2F5)3PFOCs or
(C2F5)2PF2OCs, resp.; hydrolysis of the latter gave C2F5P(O)FOCs. Treating
R3PF2 (R = C2F5, C3F7, C4F9) with MF (M = Cs, K, Na) in Et2O gave quant.

M+[R3PF3]-. Diazotization of 4-XC6H4NH2 (X = Cl, Me, NO2) and subsequent reaction with K+[R3PF3]- (R = C2F5, C3F7) gave 77-88% [4-XC6H4N2]+[R3PF3]-.

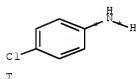
RX(40) OF 63 COMPOSED OF RX(11), RX(7), RX(10), RX(18)
 RX(40) X + T ==> S + G



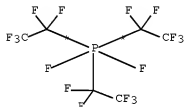
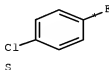
X: CM 1



X: CM 2



4
 STEPS
 →



G

RX(11) RCT X 123199-73-5
 PRO Y 352-32-9, M 91543-33-8
 NTE thermal

RX(7) RCT M 91543-33-8
 RGT J 7789-23-3 KF
 PRO O 123199-67-7
 SOL 60-29-7 Et2O

RX(10) RCT T 106-47-8

STAGE(1)

RGT V 7647-01-0 HCl, W 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(2)

RCT O 123199-67-7

SOL 7732-18-5 Water

PRO U 123199-72-4

RX(18) RCT U 123199-72-4

PRO S 352-33-0, G 91543-32-7

NTE thermal

L4 ANSWER 13 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 108:221504 CASREACT Full-text

TITLE: Electrophilic substitution in indoles. Part 15. The reaction between methylenediindoles and p-nitrobenzenediazonium fluoroborate

AUTHOR(S): Jackson, Anthony H.; Prasitpan, Noojaree; Shannon, Patrick V. R.; Tinker, Alan C.

CORPORATE SOURCE: Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK

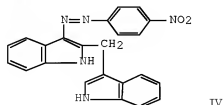
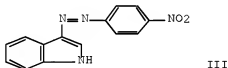
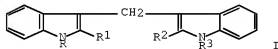
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (11), 2543-51

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

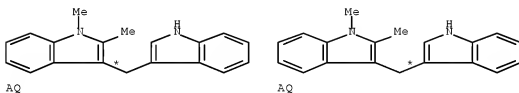
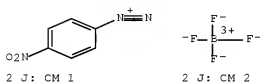
GI



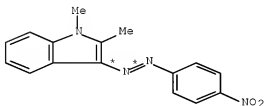
AB The preparation and substitution reaction of methylene diindoles I (R-R3 = H; R = R3 = Me, R1 = R2 = H; R = R1 = H, R2 = R3 = Me; R = R2 = R3 = H, R1 = Me)

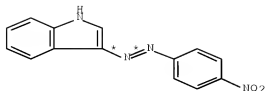
with 4-O₂NC₆H₄N₂⁺ BF₄⁻ (II) are described. Thus, indole was treated with aqueous CH₂O in AcOH to give 98% I (R-R₃ = H). Reacting the latter I with II in MeCN gave a mixture of 45% (nitrophenylazo)indole III and 39% methylenediindole IV. The displacement of indolylmethyl residues from methylenediindoles by II, and the formation of the azo coupled rearrangement product IV provides evidence that azo coupling of 3-alkylindoles to give 2,3-disubstituted indoles proceeds by initial attack at the 3-position followed by rearrangement, rather than by direct substitution at the 2-position.

RX(26) OF 378 ...2 J + 2 AQ ==> S + Y...



(26) →





Y

RX(26) RCT J 456-27-9, AQ 114648-74-7
 PRO S 114648-69-0, Y 53330-79-3
 SOL 64-17-5 EtOH, 7732-18-5 Water
 NTE 2 equiv. diazonium salt

L4 ANSWER 14 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

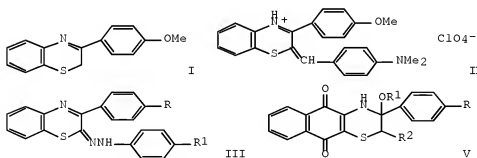
ACCESSION NUMBER: 94:48807 CASREACT Full-text
 TITLE: New dyes based on 3-arylbenzo- and
 -naphtho-1,4-thiazines

AUTHOR(S): MacKenzie, Neil E.; Thomson, Ronald H.; Greenhalgh,
 Colin W.

CORPORATE SOURCE: Dep. Chem., Univ. Aberdeen, Aberdeen, AB9 2UE, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1980), (12), 2923-32

CODEN: JCPRB4; ISSN: 0300-922X

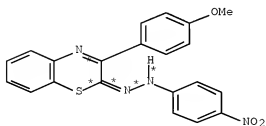
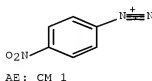
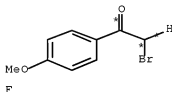
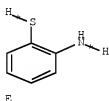
DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB 3-Aryl-2H-1,4-benzothiazines were converted into cyanine dyes by condensing their perchlorates with aldehydes, and into azo compds. by coupling with reactive diazonium salts. E.g., condensation of the perchlorate [76149-00-3] of benzothiazine I with 4-Me2NC6H4CHO [100-10-7] gave 70% blue perchlorate II [76149-01-4], the free base of which was orange, whereas I [76148-93-1] coupled with 4-MeO2CC6H4N2+SO4- [76148-96-4] to give 65% azo dye III (R = OMe, R1 = CO2Me) [76148-95-3]. The azo compds. were also obtained by

condensing arylglyoxal hydrazone bromides with 2-H₂NC₆H₄SNa [52380-58-2]. E.g., PhCOCBr:NNHPh [55716-62-6] condensed with 2-H₂NC₆H₄SNa to give 84% III (R = R₁ = H) [76148-94-2]. 2-Amino-3-mercapto-1,4-naphthoquinone (IV) [76148-76-0] condensed with *o*-bromoacetophenones to give naphthothiazinequinones. E.g., IV with BrCH₂COC₆H₄OMe-4 [2632-13-5] gave 95% naphthothiazinequinone V (R = OMe, R₁ = R₂ = H) [76148-98-6]. Attempts to dehydrate the naphthothiazinequinones gave a variety of products; reactions included extrusion of S and loss of H₂O giving indolequinones and oxidative dimerization of the quinones. Oxidation of V (R = R₁ = R₂ = H) [76148-97-5] with iodosobenzene diacetate [3240-34-4] in AcOH gave 45% V (R = H, R₁ = Et, R₂ = OAc) [76148-99-7] by an indirect Pummerer oxidation

RX(46) OF 68 COMPOSED OF RX(2), RX(16)
RX(46) E + F + AE ==> AF



RX(2) RCT E 137-07-5, F 2632-13-5
PRO A 76148-93-1
CAT 141-52-6 NaOEt

RX(16) RCT A 76148-93-1, AE 51979-06-7
PRO AF 76148-69-1
CAT 127-09-3 AcONa

L4 ANSWER 15 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 84:180173 CASREACT [Full-text](#)

TITLE: Approaches to the synthesis of
quinazolino[1,2,3]benzotriazinones

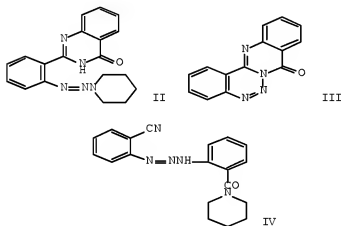
AUTHOR(S): Ahern, T. Patrick; Fong, Handrick; Vaughan, Keith
CORPORATE SOURCE: Dep. Chem., St. Mary's Univ., Halifax, NS, Can.

SOURCE: Canadian Journal of Chemistry (1976), 54(2), 290-6
CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal

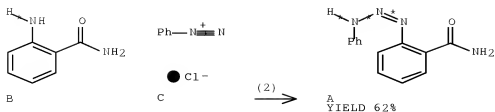
LANGUAGE: English

GI



AB The 1-(o-carboxamidophenyl)-3-aryltriazenes o-RCOC₆H₄N:NNHC₆H₄R₁-o I (R = NH₂, R₁ = H, CONH₂; R = MeO, R₁ = CONH₂) were prepared from o-H₂NC₆H₄CONH₂ and o-R₁C₆H₄N₂⁺ and reaction of o-MeO₂CC₆H₄N₂⁺ with o-H₂NC₆H₄CO₂NH₂. Reaction of I (R = MeO, R₁ = H₂NCO) with piperidine in EtOH gave 2-[2-(piperidin-1-ylazo)phenyl]quinazolin-4(3H)-one (II). Quinazolino[3,2-c][1,2,3]benzotriazin-8-one (III) was obtained from IV by cyclization, rearrangement, and further cyclization.

RX(2) OF 7 B + C ==> A



RX(2) RCT B 88-68-6, C 100-34-5
PRO A 59255-02-6

=> d his

(FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008)

L1 FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008
STRUCTURE UPLOADED

L2 FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008
L3 177 S L1 SSS FULL
L4 15 S L2 AND (DIAZONIUM SALT)
L5 15 S L3

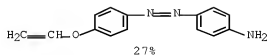
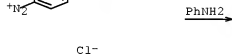
=> s L2 AND (nucleophil?)
28295 NUCLEOPHIL?
L5 13 L2 AND (NUCLEOPHIL?)

=> d scan

L5 13 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI (Vinyloxy)benzenediazonium chloride in reactions of nitrogen coupling and the exchange of the diazo group with nucleophilic reagents

RX(3) OF 9



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d ibib abs fhit 1-

YOU HAVE REQUESTED DATA FROM 13 ANSWERS - CONTINUE? Y/(N):y

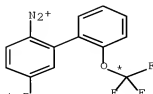
ACCESSION NUMBER: 147:406619 CASREACT [Full-text](#)
 TITLE: CF3 Oxonium Salts, O-(Trifluoromethyl)dibenzofuranium Salts: In Situ Synthesis, Properties, and Application as a Real CF3+ Species Reagent
 AUTHOR(S): Umemoto, Teruo; Adachi, Kenji; Ishihara, Sumi
 CORPORATE SOURCE: MEC Laboratory, Daikin Industries Ltd., Ibaraki, 305, Japan
 SOURCE: Journal of Organic Chemistry (2007), 72(18), 6905-6917
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB We report in situ synthesis of the first CF3 oxonium salts, thermally unstable O-(trifluoromethyl)dibenzofuranium salts, which furthermore have different counteranions (BF4-, PF6-, SbF6-, and Sb2F11-) and ring substituents (tert-Bu, F, and OCH3), by photochem. decomposition of the corresponding 2-(trifluoromethoxy)biphenyl-2'-diazonium salts at -90° to -100°. The yields markedly increased in the order of BF4- < PF6- < SbF6- < Sb2F11-. The CF3 oxonium salts were fully assigned by means of 1H and 19F NMR spectroscopy at low temperature. The CF3 salts decomposed to form CF4 and dibenzofurans. The half-life times at -60° of the C-2 tert-Bu substituted salts having different counteranions were 29 min for the BF4- salt, 36 min for the PF6- salt, 270 min for the SbF6- salt, and 415 min for the Sb2F11- salt. Half-life times at -60° for Sb2F11- salts having different C-2 substituents were 13 min for the fluoro C-2 substituted salt, 63 min for the unsubstituted salt, and 415 min for the tert-Bu C-2 substituted salt. Thus, the stability of the CF3 oxonium salts increased in the counterion order of BF4- < PF6- < SbF6- < Sb2F11- and increased in the C-2 substituent order F < H < tert-Bu, which is in accord with the increasing non- nucleophilicity of counteranions and the electron-donating effect of ring substituents. 2-Tert-Butyl-O-(trifluoromethyl)dibenzofuranium hexafluoroantimonate was successfully applied as a CF3+ species source to the direct O- and N-trifluoromethylations of alcs., phenols, amines, anilines, and pyridines under very mild conditions. Thermal decomposition of a mixture of 2-[2-(F3C)C6H4]C6H4N2+ F6Sb- and aryl- or alkylsulfonic acids, pyridine, or pyridines having an electron-withdrawing group gave CF3O or CF3N products. The trifluoromethylation mechanism is discussed and an SN2 mechanism containing the transient formation of free CF3+ is proposed. Thus, the exceedingly reactive CF3+ species can be generated much easier than the CH3+ species, contrary to the common sense that CF3+ is extremely difficult to generate in solution

RX(48) OF 381 ...AQ + CM ==> CN



AQ: CM 1



AQ: CM 2



CM

(48) →



CN
YIELD 93%

RX(48) RCT AQ 220351-08-6

STAGE(1)

SOL 75-09-2 CH2Cl2
CON 70 minutes, -90 - -100 deg C

STAGE(2)

RCT CM 62-53-3
SOL 75-09-2 CH2Cl2
CON 3 hours, -90 deg C -> -10 deg C

PRO CN 2070-47-5

NTE irradiated at 253.7nm - first stage, photochemical (first stage)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:188529 CASREACT [Full-text](#)
TITLE: Rhodium-Catalyzed Ring-Opening Reactions of
N-Boc-Azabenzonorbornadienes with Amine
Nucleophiles

AUTHOR(S): Cho, Yong-hwan; Zunic, Valentin; Senboku, Hisanori;
Olsen, Madeline; Lautens, Mark

CORPORATE SOURCE: Davenport Laboratories, Department of Chemistry,
University of Toronto, Toronto, ON, M5H 3H6, Can.
SOURCE: Journal of the American Chemical Society (2006),
128(21), 6837-6846

CODEN: JACSAT; ISSN: 0002-7863

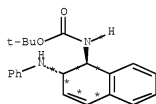
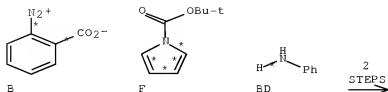
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the presence of a rhodium catalyst (5 mol %) generated in situ from [Rh(cod)Cl]₂ and (S,S')-(R,R')-C₂-ferriphos, the asym. ring-opening reaction of azabenzonorbornadienes with various aliphatic and aromatic amines proceeded with high enantioselectivity (≤ 99% ee) to give 1,2-dihydronaphthalene-1,2-diamines in high yields. In the specific case of pyrrolidine as nucleophile, Et₃NHCl was necessary as an additive for good reactivity and enantioselectivity. Addnl., a practical protocol was developed for the ring-opening of N-tert.-butoxycarbonyl-7-azabenzonorbornadiene with volatile amines at elevated temps. and standard pressure, using R₂NH.HI and (Me₂CH)₂NH. The exptl. results showed that the nature of the chiral ligand has the significant impact on the reactivity of the catalyst and the use of excess amount (2.2 equiv to Rh) of the chiral ligand plays an important role to improve the enantioselectivity in the present asym. reaction.

RX(57) OF 98 COMPOSED OF RX(2), RX(20)
 RX(57) B + F + BD ==> BE



BE
 YIELD 96%

RX(2) RCT B 1668-42-0, F 5176-27-2
 PRO G 5176-28-3
 SOL 107-06-2 ClCH2CH2Cl
 CON SUBSTAGE(1) 45 minutes, 60 deg C
 SUBSTAGE(2) 60 deg C -> room temperature

RX(20) RCT G 5176-28-3, BD 62-53-3
 PRO BE 897439-87-1
 CAT 12092-47-6 Rh COD Cl dimer, 126108-99-4 Ferrocene,
 1,1'-bis[(1S)-1-(dimethylamino)ethyl]-2,2'-
 bis(diphenylphosphino)-, (2S,2'S)-
 CON 30 hours, 80 deg C
 NTE no solvent, stereoselective

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 13 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 144:311953 CASREACT Full-text
 TITLE: Synthesis of thiazolidin-4-one derivatives on the
 basis of α -substituted thiocyanates
 AUTHOR(S): Ostapiuk, Yuri V.; Matiychuk, Vasyl S.; Obushak,
 Mykola D.
 CORPORATE SOURCE: Department of Organic Chemistry, Ivan Franko National
 University of Lviv, Lvov, 79005, Ukraine
 SOURCE: International Electronic Conferences on Synthetic
 Organic Chemistry, 5th, 6th, Sept. 1-30, 2001 and 2002
 [and] 7th, 8th, Nov. 1-30, 2003 and 2004 (2004),

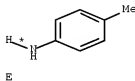
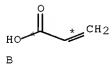
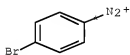
1707-1712. Editor(s): Seijas, Julio A. Molecular
Diversity Preservation International: Basel, Switz.
CODEN: 69GTGO
Conference; (computer optical disk)
English

DOCUMENT TYPE:
LANGUAGE:
GI

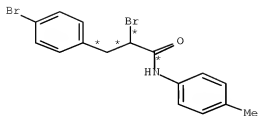
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A conference. 2-Bromo-3-(4-bromophenyl)propionic acid has been obtained by interaction of 4-bromobenzenediazonium bromide with acrylic acid (catalyst - CuBr). 2-Bromo-3-(4-bromophenyl)propionic acid has been used for the synthesis of amides, e.g. I. 5-(4-Bromobenzyl)-2-imino-3-R1-thiazolydin-4-ones, e.g. II, have been obtained on account of intramol. reaction by the nucleophilic substitution of bromine by thiocyanate ion of these amides. By the reaction of arenediazonium chlorides with acrolein (catalyst - CuCl₂) the 3-aryl-2-chloropropanals have been synthesized. By the interaction of 3-aryl-2-chloropropanals with thiourea, 5-R-benzyl-2-aminothiazoles, e.g. III, have been obtained, that have been transformed to corresponding N-(5-R-benzylthiazol-2-yl)-2-chloroacetamides, e.g. IV, by action of chloroacetyl chloride. N-(5-R-benzylthiazol-2-yl)-2-chloroacetamides are ring closing under action of thiocyanate ion and form 3-substituted 2-iminothiazolydin-4-ones, e.g. V. By alkylation of benzothiazole-2-thiol and morpholine with N-(5-R-benzylthiazol-2-yl)-2-chloroacetamides, corresponding N-(5-R-benzylthiazol-2-yl)-2-(benzothiazol-2-yl)thioacetamides, e.g. VI, and 4-(5-R-benzylthiazol-2-yl)-4- morpholinecarboxamide have been obtained.

RX(35) OF 91 COMPOSED OF RX(1), RX(2)
RX(35) A + B + E ==> F



2
STEPS
→



F
YIELD 67%

RX(1) RCT A 2028-62-2, B 79-10-7
PRO C 857813-94-6
CAT 7787-70-4 CuBr
NTE Meerwein arylation

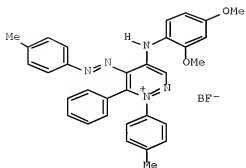
RX(2) RCT C 857813-94-6
STAGE(1)
RGT G 7719-09-7 SOC12

STAGE(2)
RCT E 106-49-0

PRO F 879497-64-0

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 13 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:219222 CASREACT Full-text
TITLE: Formation of pyridazinium salts by azo coupling of
N-substituted 3-amino-1-phenylbut-2-en-1-ones and
diazonium salts
AUTHOR(S): Simunek, Petr; Peskova, Marketa; Bertolasi, Valerio;
Lycka, Antonin; Machacek, Vladimir
CORPORATE SOURCE: Department of Organic Chemistry, University of
Pardubice, Pardubice, 53210, Czech Rep.
SOURCE: European Journal of Organic Chemistry (2004), (24),
5055-5063
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

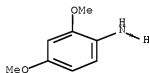


I

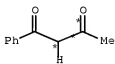
AB Treatment of 3-(2,4-dimethoxyphenylamino)- and 3-methylamino-1-phenylbut-2-en-1-ones with some benzenediazonium tetrafluoroborates gave 1,4,5,6-tetrasubstituted pyridazinium tetrafluoroborates, e.g., I. The pyridazinium salts have been identified by X-ray anal. and by their ^1H , ^{13}C , ^{15}N , ^{11}B , and ^{19}F NMR spectra. Their formation is most probably the result of nucleophilic attack on the carbonyl carbon by the nitrogen of the hydrazone group and subsequent dehydration.

RX(7) OF 10 COMPOSED OF RX(1), RX(2)

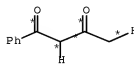
RX(7) 2 A + 2 B + 3 E ==> F + G



2 A



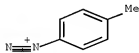
B



B

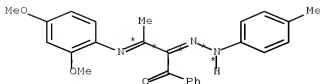


3 E: CM 1



3 E: CM 2

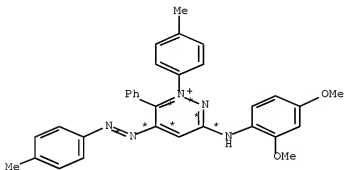
2
STEPS
→



F
YIELD 79%



G: CM 1
YIELD 17%



G: CM 2
YIELD 17%

RX(1) RCT A 2735-04-8, B 93-91-4
PRO C 387832-31-7
SOL 108-88-3 PhMe
CON 3 hours, reflux

RX(2) RCT C 387832-31-7, E 459-44-9
RGT H 127-09-3 AcONa
PRO F 843613-91-2, G 843613-95-6
SOL 75-09-2 CH2Cl2
CON 72 hours, room temperature

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 142:176480 CASREACT [Full-text](#)

TITLE: 2-Alkyl-1,2,3,4-benzotetrazinium tetrafluoroborates:
Their reaction with nucleophiles

AUTHOR(S): Lipilin, Dmitry L.; Smirnov, Oleg Y.; Churakov,
Aleksandr M.; Strelenko, Yuri A.; Tyurin, Aleksei Y.;
Ioffe, Sema L.; Tartakovsky, Vladimir A.

CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry, Russian
Academy of Sciences, Moscow, 119991, Russia

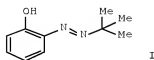
SOURCE: European Journal of Organic Chemistry (2004), (23),
4794-4801

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

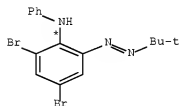
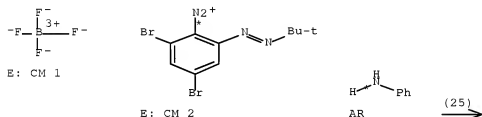
DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



AB Treatment of 2-alkyl-1,2,3,4-benzotetrazinium tetrafluoroborates with a variety nucleophiles, at room temperature, resulted in elimination of an N2 mol. to afford ortho-substituted azobenzenes, e.g., I. This reaction could be suitable for mild phenylation of carboxylic acids and other compds. containing active hydrogen. A plausible reaction pathway for the reaction is discussed.

RX(25) OF 39 E + AP ==> AS



YIELD 97%

RX(25) RCT E 832076-98-9, AR 62-53-3
PRO AS 832077-20-0
SOL 75-09-2 CH2Cl2
CON 10 minutes, 20 deg C

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS

L5 ANSWER 6 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 139:214429 CASREACT Full-text

TITLE: Synthesis of azo-coupled itaconic acid anhydride and its reactions with nucleophiles

AUTHOR(S): Prabhu, P. J.; Bhise, N. B.; Dave, M. A.

CORPORATE SOURCE: Department of Chemistry, K.J. Somaiya College of Science and Commerce, Mumbai, 400 077, India

SOURCE: Asian Journal of Chemistry (2003), 15(2), 634-638

CODEN: AJCHEW; ISSN: 0970-7077

PUBLISHER: Asian Journal of Chemistry

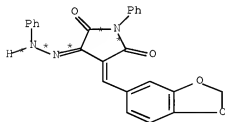
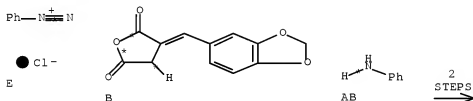
DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3,4-Methylenedioxy-benzylidene succinic anhydride was condensed with diazonium salts of various aromatic amines to form hydrazones or dyes which were further treated with nucleophiles like 10% NaOH and NaBH₄ to give various pyrazolinone derivs., resp. and cyclic imide derivs. of the corresponding hydrazones. The antibacterial and antifungal activities of some the products are also reported.

RX(24) OF 45 COMPOSED OF RX(2), RX(14)

RX(24) E + B + AB ==> AC



AC
YIELD 64%

RX(2) RCT E 100-34-5

STAGE(1)

RGT G 7647-01-0 HCl, H 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 15 minutes, 0 deg C

STAGE(2)
RCT B 99971-42-3
SOL 67-64-1 Me2CO
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, 0 deg C

PRO F 587881-56-9

RX(14) RCT F 587881-56-9, AB 62-53-3

STAGE(1)
SOL 64-17-5 EtOH
CON 4 - 5 hours, reflux

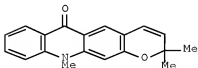
STAGE(2)
CAT 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature

PRO AC 587881-78-5

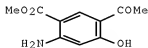
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 139:85518 CASREACT [Full-text](#)
TITLE: Regioselective synthesis of demethoxyisoacronycine
involving nucleophilic addition to benzyne
AUTHOR(S): Rudas, Monika; Nyerges, Miklos; Toke, Laszlo;
Groundwater, Paul W.
CORPORATE SOURCE: Research Group of the Hungarian Academy of Sciences,
Department of Organic Chemical Technology, Technical
University of Budapest, Budapest, H-1521, Hung.
SOURCE: Heterocycles (2003), 60(4), 817-824
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



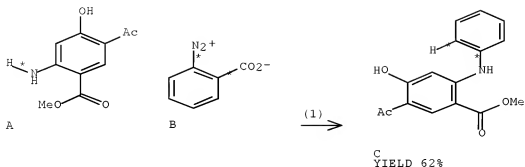
I



II

AB Demethoxyisoacronycine (I) was prepared in seven steps using the nucleophilic addition of aniline derivative II to benzyne as a key step.

RX(1) OF 32 A + B ==> C...



RX(1) RCT A 71407-97-1, B 1608-42-0
 PRO C 250644-93-0
 SOL 75-09-2 CH2Cl2
 CON reflux

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 138:4399 CASREACT [Full-text](#)

TITLE: Synthesis and Transformations of
 2-Hydroxy-3-aryldiazo-1,4-naphthoquinones

AUTHOR(S): Romanyuk, A. L.; Polishchuk, O. P.; Litvin, B. L.;
 Ganushchak, N. I.

CORPORATE SOURCE: Franko State University, Lvov, Ukraine

SOURCE: Russian Journal of General Chemistry (Translation of
 Zhurnal Obshchei Khimii) (2002), 72(2), 251-254
 CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: MAIK Nauka/Interperiodica Publishing

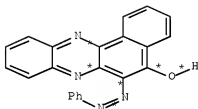
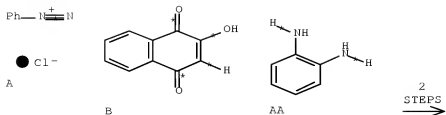
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 2-hydroxy-3-aryldiazo-1,4-naphthoquinones was prepared by coupling of 2-hydroxy-1,4-naphthoquinone with aryldiazonium chlorides. The reactivity of the products toward electrophilic and nucleophilic agents was studied. In reaction with o-phenylenediamine they give condensation products, the corresponding benzo[a]phenazines.

RX(15) OF 17 COMPOSED OF RX(1), RX(12)

RX(15) A + B + AA ==> AB



AB
YIELD 63%

RX(1) RCT A 100-34-5

STAGE(1)

RGT D 144-55-8 NaHCO3
 SOL 7732-18-5 Water
 CON 0 - 5 deg C

STAGE(2)

RCT B 83-72-7
 RGT D 144-55-8 NaHCO3
 SOL 7732-18-5 Water
 CON - 1.5 hour

STAGE(3)

RGT E 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO C 476682-15-2

RX(12) RCT AA 95-54-5, C 476682-15-2
 PRO AB 68839-40-7
 SOL 64-17-5 EtOH
 CON 2 hours, reflux

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

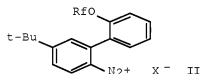
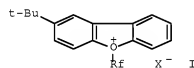
L5 ANSWER 9 OF 13 CASREACT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 130:168232 CASREACT [Full-text](#)
 TITLE: Preparation of O-(perfluoroalkyl)dibenzofuranium salts

as perfluoroalkylating agents and their intermediates
 such as (perfluoroalkoxy)biphenyldiazonium salts
 Umemoto, Teruo; Adachi, Kenji; Ishihara, Sumi
 Daikin Industries Ltd., Japan
 PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 Patent
 Japanese

INVENTOR(S):
 PATENT ASSIGNEE(S):
 SOURCE:
 DOCUMENT TYPE:
 LANGUAGE:
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906389	A1	19990211	WO 1998-JP3416	19980730
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1013651	A1	20000628	EP 1998-935301	19980730
EP 1013651	B1	20070530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 363477	T	20070615	AT 1998-935301	19980730
US 6239289	B1	20010529	US 2000-463706	20000215
PRIORITY APPLN. INFO.:			JP 1997-207901	19970801
			WO 1998-JP3416	19980730

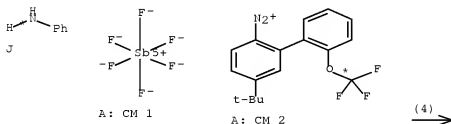
OTHER SOURCE(S): MARPAT 130:168232
 GI



AB O-(Perfluoroalkyl)dibenzofuranium salt derivs. represented by general formula (I; Rf is perfluoroalkyl being 1 to 10 carbon atoms; and X- is a conjugate based of a Bronsted acid) are prepared by cyclization of (perfluoroalkoxy)biphenyldiazonium salts (II; Rf and X- are defined as above) and are used as perfluoroalkylating agents for perfluoroalkylation of nucleophiles containing O or N, e.g. amines and alcs. When the O-(perfluoroalkyl)dibenzofuranium salt derivs. are used as perfluoroalkylating agents, they permit high-yield perfluoroalkylation, and are applicable to a wide range of compds. and inhibited in self-decomposition as to be relatively stable. The presence of tert-Bu at 5-position improves the stability of I and thereby usefulness of I as perfluoroalkylating agents. Thus, a solution of 7.17 g 2-amino-5-tert-butyl-2'-(trifluoromethoxy)biphenyl in 46 mL Et2O was cooled to -78° with stirring, followed by adding 6.47 g nitrosonium hexafluoroantimonate (ON+SbF6-), and the resulting mixture was warmed to 10° over 3 h in an warm bath, while adding 10 mL Et2O when temperature reached to

5°, to give 58% II (Rf = CF₃, X- = SbF₆⁻) (III). A CCl₂D₂ solution of 6.5 mg III in a Pyrex NMR tube was cooled to -106° and irradiated by a high pressure Hg lamp (400 W and 253.7 nm) for 45 min to give I (Rf = CF₃, X- = SbF₆⁻) (IV) 87, 5-tert-butyl-2-fluoro-2'-(trifluoromethoxy)biphenyl 8, and 5-tert-butyl-2-chloro-2'-(trifluoromethoxy)biphenyl 3% according to ¹⁹F- and ¹H-NMR anal. at -80°. When the temperature was gradually raised to -30°, IV completely decomposed to CF₄ and 2-tert-butylbenzofuran. To the cold (-99° to -90°) reaction mixture similarly prepared were added variety of alcs. and amines. When phenecyl alc. was added at -90°, the resulting mixture was warmed to -10° over 3 h to give 80% phenecyl trifluoromethyl ether. Although in general, diazonium salts are explosive in nature, III has .apprx.27° higher decomposition temperature (84.7-85.8°) compared to that of the 4-tert-Bu regioisomer (m.p. 58-60°) and can be handled at room temperature, and safely stored and transported.

RX(4) OF 9 J + A ==> K



RX(4) RCT J 62-53-3, A 220351-03-6
PRO K 2070-47-5
SOL 75-09-2 CH2Cl2
NTE two-step reacti

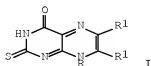
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 13 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 110:192508 CASREACT [Full-text](#)
TITLE: Pteridines. Part LXXXVII. Synthesis and properties of 8-substituted 2-thiolumazines
AUTHOR(S): Huebsch, Walter; Pfleiderer, Wolfgang
CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: Helvetica Chimica Acta (1988), 71(6), 1379-91

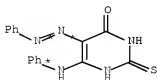
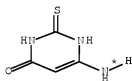
DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: HCACAV; ISSN: 0018-019X
Journal
English



AB 2,8-Dihydro-2-thioxopteridin-(3H)-ones I (R = Me, CH₂CH₂OH, Ph; R₁ = H, Me, Ph) and their S-Me derivs. have been synthesized by condensation of 5-amino-6-(substituted amino)-1,2-dihydro-2-thioxopyrimidin-4(3H)-ones and the S-Me derivs. with R₁COCOR₁. The presence of a quinonoid cross-conjugated π -electron system makes this type of compound susceptible to nucleophilic addns. in position 7, which leads to intramol. and intermol. covalent adducts.

RX(43) OF 124 COMPOSED OF RX(3), RX(10)
RX(43) A + G + P ==> W



YIELD 89%

RX(3) RCT A 1004-40-6, G 142-04-1
PRO H 98421-02-4

RX(10) RCT H 98421-02-4, R 190-34-5
 RGT N 1310-73-2 NaOH
 PRO W 120270-10-2
 SOL 7732-18-5 Water, 64-17-5 EtOH

L5 ANSWER 11 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

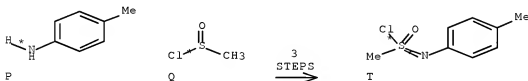
ACCESSION NUMBER: 100:155992 CASREACT [Full-text](#)
 TITLE: Reactions of (aryloxy)oxosulfonium ylides with
 carbonyl compounds
 AUTHOR(S): Okuma, Kentaro; Nakanishi, Kazuto; Ohta, Hiroshi
 CORPORATE SOURCE: Dep. Chem., Fukuoka Univ., Fukuoka, 814-01, Japan
 SOURCE: Journal of Organic Chemistry (1984), 49(8), 1402-7
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB (Aryloxy)oxosulfonium salts and alkylolithiums give ylides which add to carbonyl compds. to give β -(aryloxy) sulfones (I) β -(aryloxy) sulfones (II), and α,β -unsatd. or β,γ -unsatd. sulfones in 1.4-17.9, 1.2-7.2, and 4.5-13.5% yields, resp. The ylides reacted with the carbonyl compds. to give betaines which formed unusual 4-membered cyclic alkoxyoxosulfonium salts containing aryloxy anions. The aryloxy anions thus formed attacked the β -C of these salts to give I; the aryloxy anions, which might be formed by autoxidn., also attack the β -C of these salts to give II. Deprotonation at C(α) or C(γ) by these anions gave the unsatd. sulfones. This is the first example in which an ylide reacts with carbonyl compds. to give sulfones via a 4-membered cyclic alkoxyoxosulfonium salt which was formed in an intramol. SN2 reaction. To yields of unsatd. sulfones were raised to 35-60% in a one-pot reaction.

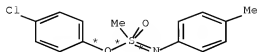
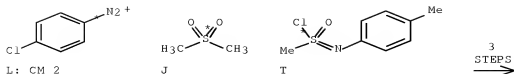
RX(48) OF 48 COMPOSED OF REACTION SEQUENCE RX(12), RX(21), RX(13)
 AND REACTION SEQUENCE RX(9), RX(1), RX(13)

... E + Q ==> T...
 ... L + J + T ==> U



L: CM 1

START NEXT REACTION SEQUENCE



U
YIELD 77%

RX(12) RCT P 106-49-0, Q 676-85-7
 PRO R 19977-37-8
 CAT 121-44-8 Et3N

 RX(21) RCT R 19977-37-8
 RGT AF 7782-50-5 Cl2
 PRO T 89278-81-9

 RX(9) RCT L 673-41-6, J 67-71-0
 PRO A 73040-88-7

 RX(1) RCT A 73040-88-7
 PRO B 106-48-9
 CAT 104-87-0 4-MeC6H4CHO

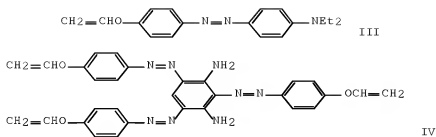
 RX(13) RCT T 89278-81-9, B 106-48-9
 PRO U 89278-82-0

L5 ANSWER 12 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 97:162482 CASREACT [Full-text](#)

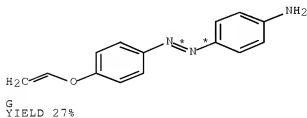
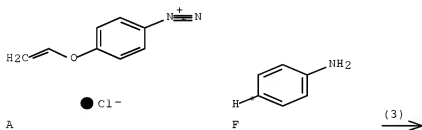
TITLE: (Vinyloxy)benzenediazonium chloride in reactions of
 nitrogen coupling and the exchange of the diazo group
 with nucleophilic reagents
 AUTHOR(S): Stepanova, Z. V.; Grebneva, P. I.; Skvortsova, G. G.
 CORPORATE SOURCE: Inst. Org. Khim., Irkutsk, USSR
 SOURCE: Zhurnal Organicheskoi Khimii (1982), 18(8), 1711-15
 CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB 4-CH₂:CHOC₆H₄N₂+Cl⁻ (I) underwent azo coupling with PhNH₂, PhNMe₂, PhNEt₂, and 1,3-C₆H₄(NH₂)₂ (II) to give, e.g., III; with II di- and tri-coupling products (e.g., IV) were also obtained. Reactions with HgCl₂ and CuCl were also studied; with CuCN I and its m-isomer gave the corresponding nitriles.

RX(3) OF 9 A + F ==> G



RX(3) RCT A 34645-14-4, F 62-53-3
 PRO G 83300-43-0

ACCESSION NUMBER: 83:164108 CASREACT Full-text
 TITLE: Nucleophilic displacement of aromatic
 fluorine. I. Synthesis of benzisoxazoles
 AUTHOR(S): Walser, Armin; Flynn, Thomas; Fryer, R. Ian
 CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ,
 USA
 SOURCE: Journal of Heterocyclic Chemistry (1974), 11(6), 885-8
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English

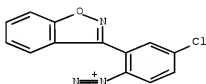
GI For diagram(s), see printed CA Issue.

AB The quinazoline 3-oxides I (R = H, Cl) convert to the
 benzisoxazoloquinazolines II by heating in Ac₂O. The dihydroquinazoline-3-
 oxides III underwent aromatization under the same conditions. Hydrolysis of I
 or II gave the 3-(2-aminophenyl)benzisoxazoles IV which could be rearranged to
 the 3-(2-hydroxyphenyl)indazoles V with hydride. Possible mechanisms are
 discussed.

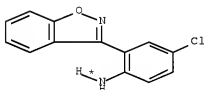
RX(12) OF 39 ...T + H ==> U



T: CM 1

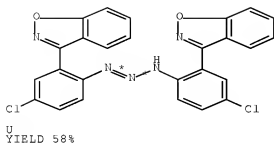


T: CM 2



N

(12) →



RX(12) RCT T 340203-43-2, N 55076-00-1
PRO U 55076-03-4

=> log off
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
STN INTERNATIONAL LOGOFF AT 10:10:24 ON 20 OCT 2008